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Reply to "Comment on 'Existence of internal modes of sine-Gordon kinks' "

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In this reply to the comment by C. R. Willis, we show, by quoting his own statements, that the simulations reported in his original work with Boesch [Phys. Rev. B **42**, 2290 (1990)] were done for kinks with nonzero initial velocity, in contrast to what Willis claims in his paper. We further show that his alleged proof, which assumes among other approximations that kinks are initially at rest, is not rigorous but an approximation. Moreover, there are other serious misconceptions which we discuss in our paper. As a consequence, our result that quasimodes do not exist in the sG equation [Phys. Rev. E **62**, R60 (2000)] remains true.

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I. INTRODUCTION

In his paper [1], Willis claims that in [2] he used a "rigorous" projection operator collective variable formalism for nonlinear Klein-Gordon equations to "prove" the continuum sine-Gordon (sG) equation has a long-lived quasimode whose frequency $\omega_s = 1.004$ is in the continuum just above the lower phonon band edge with a lifetime $(1/\tau_s) = 0.003\Gamma_0$. In [3] we performed two numerical investigations which show that neither intrinsic internal modes nor quasimodes exist in contrast to previous results. Willis further claims that he "proves" that our first numerical investigation could not possibly observe the quasimode in principle and our second numerical investigation actually demonstrates the existence of the sG quasimode. He states that his analytic calculations and verifying simulations were performed for a stationary sine-Gordon soliton at the origin, but that we explained our analytic calculations and confirming simulations in terms of the Doppler shift of the phonons when stationary sine-Gordon solitons have a zero Doppler shift. In the following we argue that his paper is irrelevant because the results Willis refers to in [2] were obtained for *moving kinks* (which we prove by quoting statements from [2]), and because his alleged "proof" is not a mathematical proof but an approximate calculation as any collective coordinate theory [4].

II. ON THE NONSTATIONARITY OF KINKS

After carefully reading their paper [2] several times, we are afraid that Willis's paper suffers from misconceptions. Quoting literally from [2], p. 2296, first paragraph beginning after Eq. (3.2), it reads: "We impose initial conditions in our simulations in two different ways. The first way is by specifying the field [...] thus giving the equilibrium kink a nonzero initial velocity." Subsequently, three out of four figures of the paper refer to this type of simulation. For instance, the caption of Fig. 1 reads: "The initial condition for $t=0$ is a kink with velocity determined by specifying the kink shape at … ." Therefore, in spite of Willis's claims that their simulations were for stationary kinks, that is not the case, and he cannot dismiss our explanation of his observations based on this. Kinks moved in his simulations and correspondingly their phonon spectra were shifted, as we explained in [3].

III. MISCONCEPTIONS IN THE PRECEDING PAPER

In his paper [1] Willis claims:

(i) "What they measured was the phonon absorption spectrum of the linearized sine-Gordon (sG) equation … ." This is simply not correct. We simulated the full sG equation: in page R61 of [3], in the beginning of Sec. III, this is perfectly clear: "We have computed the numerical solution of the perturbed sG equation… ." We never linearized anything and worked with the full equation.

(ii) "Consequently, their two equations of motion for $P(t)$ and $l(t)$, which they state are the 'basis of their theoretical analysis' of Ref. [3] have no relevance to our analytic derivation and confirming simulations." This is not correct. Actually, those equations are the way we find that, were there any internal modes or quasimodes in the kink, they would be excited parametrically by the ac driving. In spite of his claim that he "proved in Sec. III that an ac driver cannot create a sG quasimode," we have shown, by means of those equations, that parametric excitation at half the frequency of the

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mode must be observed. We refer the interested reader to [5–7] to learn more about this effect. On this issue, it is particularly important to realize the inconsistencies in Willis's reasoning: Just after Eq. (16) of [1] Willis claims: "Thus an ac force field cannot possibly excite a phonon mode. Consequently, their first numerical investigation in Ref. [3] could not possibly detect the presence of the sG quasimode and thus it has no relevance to the existence or nonexistence of the sG quasimode." If this were true (which it is not), Willis would be forced to conclude that a biharmonic force $f(t)=-[\epsilon_1 \cos(\omega t)+\epsilon_2 \cos(2\omega t+\theta)]$ is also unable to excite the phonons. But this is not the case: On the contrary, Willis has recently studied [8], by using the same approximate method that he developed in 1990, the action of this biharmonic force and dissipation on the ratchet motion of the kink. In this paper, he claims: "We use a rigorous collective variable for nonlinear Klein-Gordon equations to prove that the rectification of the current is due to the excitation of an internal mode $\Gamma(t)$, which describes the oscillation of the slope of the kink, and due to a dressing of the bare kink by the ac driver." In Willis's own words, dressing of the kinks means phonons excited in the system, in contradiction with his remark on our work. We also note that Willis's discussion of our theoretical treatment contains misconception about "exact analytical calculations" in his earlier paper, which unfortunately are not exact (cf. Sec. V below).

(iii) "The simulations and analysis by the authors in Ref. [3] were done for an appreciably discrete sG equation." This is not correct. Our discretization was of the same order as that of [2]: 0.05 in our case, 0.02 in theirs [cf. [2], p. 2296, below Eq. (3.1)]. If ours is irrelevant, so is the one in [2], and vice versa.

(iv) On the other hand, Willis does not trust our numerical simulations and explicitly refers to the "flawed design of their (ours in [3]) simulation," claims that all we observe in Fig. 2 of [3] is "a complicated interference pattern," arising from "reflection of phonons at the boundary at time 200." We were fully aware of the possibility of phonon reflection at the boundaries, this being the reason why we used free boundary conditions, to minimize this effect. Furthermore, we did not trust a visual inspection of our Fig. 2 as he does, and carried out a Fourier analysis of the time evolution of the kink width, finding only phonons (as Willis points out, present in the system due to emission and reflection). We did not find any Fourier peak arising from a hypothetical "quasimode," in spite of the fact that the author of the paper concedes that "the first 200 s [actually, time units] of their simulation of the width $l(t)$ [actually, the simulation was for the full sine-Gordon equation, not of the width] gives a very good representation of the sG quasimode." How can it be then that it does not show up in the Fourier spectra, which we report in the paragraph below Fig. 2?

IV. ON FURTHER EVIDENCE ON THE NONEXISTENCE OF QUASIMODES

We would like to refer the reader to additional research that has significantly advanced the subject. Indeed, one of us (N.R.Q.) has published a very relevant investigation on this subject [9], showing that the spectrum mentioned in the paper, see Eq. (15), and which we used in our own paper [Eq. (15) of [3]] is not correct, and in turn the parentheses should read $(n-1)\pi/L$ for small n/L. This paper is very pertinent to this discussion because the author of the paper seems to be very worried that we are not aware of the "phonon dressing" of the kink. This work of Quintero and Kevrekidis is the best way to understand what are the consequences of the phonons on the kink behavior.

Furthermore, there was only one other paper in the literature that observed something similar to a "quasimode" [10], in fact using simulations of kinks driven by constant forces. This only independent confirmation of the "quasimode" was also proven wrong by us in [11]. In this case, it is not a matter of simulations and how they measured the "quasimode": In the above reference we showed that the analytical calculations in this other paper were not correct. We encourage the reader to take this further report on the absence of quasimodes into account.

V. ON THE APPROXIMATE CHARACTER OF COLLECTIVE COORDINATE THEORIES

Finally, Willis does not seem to be informed about the nature and rigor of collective coordinate calculations. He states in the abstract that "prove the continuum sine-Gordon equation has a long lived quasimode… ." Unfortunately and contrary to his belief, collective coordinate calculations cannot prove anything in the mathematical sense, in so far as they are approximate. Even if he tries to keep his calculation (which, by the way, he reproduces literally from [2], therefore adding no new evidence at all in favor of his claims) exact, he cannot, and he has to make a number of approximations including two linearizations and assuming X and its derivative to be exactly zero (see p. 2293 of [2], 2nd paragraph on the right). Willis goes as far as claiming: "their Eq. (3) for $l(t)$ is incorrect because it contains none of the many terms proportional to $\chi(t)$ that appear in the exact equation of motion… ." Our equation is completely correct, consistent with our derivation, and confirmed by numerical simulations. Our result is different from his simply because neither of them is exact. They begin with different *ansätze* and subsequently lead to different *approximate* equations. Collective coordinate and related calculations are interesting, often times very accurate and useful, but by no means exact and, mathematically speaking, constitute no proof. Indeed, it has been shown that such a procedure may lead to wrong predictions: For a detailed discussion, see [4].

In this respect, we want to stress that when Willis uses the paper [12] in favor of his argument, it is again an approximate result and a conjecture. It is true that Kälbermann calculates some solutions analytically, but he has to resort to numerical simulations to make his point. In addition, the relationship of Kälbermann's "wobble solution" with Willis's "quasimode" is dubious at best: Kälbermann finds a continuum of such possible quasimodes, which is not surprising because his wobble solution is a combination of a kink and a breather, and therefore is a one-parameter family of solutions; a longer discussion of this work is out of the scope of this paper, but we want to stress that he never finds a specific quasimode as Willis claims, and Kälbermann's only example has a frequency below the phonon band, very different from Willis's quasimode. Furthermore, this wobble is, in Kälbermann's own words, only "apparently stable" and all he can be positive about is that "the kink appears to be decaying to a wobble." Therefore, there is no such thing as a mathematical proof of the existence of "quasimodes" in this paper either.

VI. CONCLUSION

Based on all the arguments summarized above, we are afraid that the preceding paper [1] contains misconceptions about our work. Willis' work did not deal with stationary kinks, the simulations in Ref. [2] are as discrete as ours, collective coordinate theories are not rigorous mathematical proofs, there are further developments on this question, and Willis misreads our paper [3]. Therefore, Willis's paper does not change our conclusions, and our result that quasimodes do not exist in the sG equation [3] stands in its own right.

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[1] C. R. Willis, preceding paper.
[2] R. Boesch and C. R. Willis, Phys. Rev. B **42**, 2290 (1990).
[3] N. R. Quintero, A. Sánchez, and F. G. Mertens, Phys. Rev. E **62**, R60 (2000).
[4] A. Sánchez and A. R. Bishop, SIAM Rev. **40**, 579 (1998).
[5] N. R. Quintero, A. Sánchez, and F. G. Mertens, Phys. Rev. Lett. **84**, 871 (2000).
[6] N. R. Quintero, A. Sánchez, and F. G. Mertens, Phys. Rev. E **62**, 5695 (2000).
[7] N. R. Quintero, A. Sánchez, and F. G. Mertens, Phys. Rev. E **64**, 046601 (2001).
[8] C. R. Willis and M. Farzaneh, Phys. Rev. E **69**, 056612 (2004).
[9] N. R. Quintero and P. G. Kevrekidis, Phys. Rev. E **64**, 056608 (2001).
[10] E. Majernikova, Y. B. Gaididei, and O. M. Braun, Phys. Rev. E **52**, 1241 (1995).
[11] N. R. Quintero, A. Sánchez, and F. G. Mertens, Eur. Phys. J. B **19**, 107 (2001).
[12] G. Kälbermann, J. Phys. A **37**, 11603 (2004).